Computing PI, Wiener and Szeged Indices of some Nanotubes and Nanotori

Ali Reza Ashrafi

Department of Mathematics, Faculty of Science, University of Kashan, Kashan, Iran

ABSTRACT

Let G be a graph. The Wiener index of G is defined as $W(G) = 1/2\sum_{\{x,y\}\subseteq V(G)}d(x,y)$, where V(G) is the set of all vertices of G and for $x,y \in V(G)$, d(x,y) denotes the length of a minimal path between x and y. The Padmakar–Ivan (PI) index of G is defined as $PI(G) = \sum[n_{eu}(e|G)+ n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u and summation goes over all edges of G. Let e be an edge of G, $N_1(e|G)$ be the number of vertices of G lying closer to one end of e and $N_2(e|G)$ be the number of vertices of G lying closer to the other end of e. Then the szeged index of the graph G is defined as $Sz(G) = \sum_{e\in E(G)}N_1(e|G)N_2(e|G)$, where E(G) is the set of all edges of G.

In this talk we present our recent works on computing Wiener, PI and Szeged indices of some nanotubes and nanotori.

Keywords: Nanotube, nanotori, Wiener index, PI index, szeged index.

References

1. M. V. Diudea, M. Stefu, B. Pârv and P. E. John, Wiener Index of Armchair Polyhex Nanotubes, *Croat.* Chem. Acta, **77**(1-2)(2004) 111-115.

2. P. E. John and M. V. Diudea, Wiener Index of Zig-zag Polyhex Nanotubes, *Croat.* Chem. Acta, **77**(1-2)(2004) 127-132.

3. Sh. Yousefi and A.R. Ashrafi, An Exact Expression for the Wiener Index of a Polyhex Nanotorus, MATCH Commun. Math. Comput. Chem., **56**(1)(2006), 169-178.

4. A.R. Ashrafi and A. Loghman, PI Index of Zig-Zag Polyhex Nanotubes, MATCH Commun. Math. Comput. Chem., **55**(2)(2006), 447-452.

5. A.R. Ashrafi and A. Loghman, PI Index of $TUC_4C_8(S)$ Carbon Nanotubes, J. Comput. Theor. Nanosci. (In press).

6. A.R. Ashrafi and F. Rezaei, PI Index of Polyhex Nanotori, MATCH Commun. Math. Comput. Chem. (In press).